

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 93.1 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.97e-01

Confidence level: 6.87e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Thidiazuron</div> <div>Measured: 110</div> <div>Predicted: 141</div>	<div>Image not found</div> <div>Diethyl phthalate</div> <div>Measured: 69.2</div> <div>Predicted: 102</div>	<div>Image not found</div> <div>Dioxacarb</div> <div>Measured: 39.8</div> <div>Predicted: 124</div>
<div>Image not found</div> <div>Oxycarboxin</div> <div>Measured: 95.5</div> <div>Predicted: 175</div>	<div>Image not found</div> <div>Carboxin</div> <div>Measured: 257</div> <div>Predicted: 210</div>	